pl12 Intermolecular interactions involving halogen substituents. I. Csöregh, Department of Structural Chemistry, Arrhenius Laboratory, Stockholm University, S-106 91 Stockholm, Sweden.

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Investigation of the characteristic behaviour of different functional groups and their influence on the realized crystal structures, is of great interest in crystal engineering, and for the design of organic solids with desired properties. Most research efforts in the past have been concentrated on using OH···O and NH···O hydrogen bonds between complementary functionalities as supramolecular design principle, and it has been shown that certain key binding motifs exist. Weaker interactions than conventional hydrogen bonds have also proved to be capable of decisevely influencing the packing arrangement in molecular crystals. Halogen substituents, in general, are often in a situation to make short intermolecular contacts with a variety of other atoms, owing to their exposed position in many molecules. Halogens covalently bonded to carbon are known to form short contacts to halogens, but also to hydrogen, nitrogen, oxygen, sulphur and aryl π electron clouds. All these connections may control crystal packing to varying degrees. Comparison of crystal structures of analogous compounds, differing only in the halogen substituents, are expected to give some hints about the role different halogens may play in formation of organic solids. The discussion will be based on results from our investigations as well as on literature data.

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